=> file registry
FILE 'REGISTRY' ENTERED AT 10:45:40 ON 19 FEB 2008
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STRUCTURE FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7 DICTIONARY FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> file caplus
FILE 'CAPLUS' ENTERED AT 10:45:42 ON 19 FEB 2008
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FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8 FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

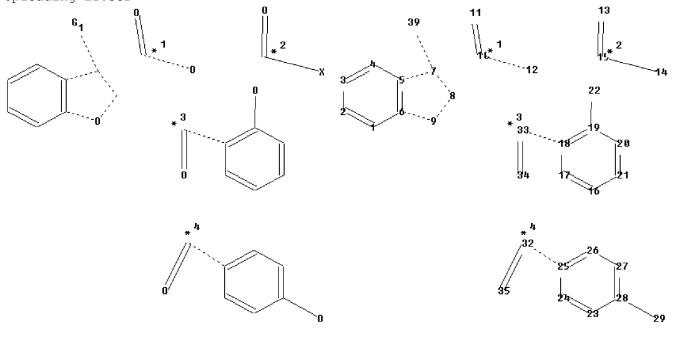
L29 1 SEA FILE=CAPLUS ABB=ON PLU=ON L23 AND L26

L30 3 SEA FILE=CAPLUS ABB=ON PLU=ON (L27 OR L28 OR L29)

=> d stat que L31 L1 ST

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation: Uploading L1.str



chain nodes :

10 11 12 13 14 15 22 29 32 33 34 35 39

ring nodes :

1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 28

chain bonds :

7-39 10-12 10-11 13-15 14-15 18-33 19-22 25-32 28-29 32-35 33-34

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 16-17 16-21 17-18 18-19 19-20

20-21 23-24 23-28 24-25 25-26 26-27 27-28

exact/norm bonds :

5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-35

33-34

exact bonds :

14 - 15

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21 \quad 23-24 \quad 23-19 \quad 20-21 \quad 23-24 \quad$

28

24-25 25-26 26-27 27-28

G1:[*1],[*2],[*3],[*4]

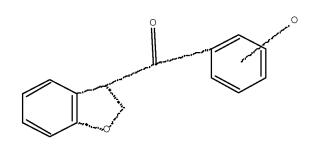
Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom

19:Atom 20:Atom 21:Atom

22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS 33:CLASS 35:CLASS 39:CLASS

L5 8858 SEA FILE=REGISTRY SSS FUL L1 L9 STR



Structure attributes must be viewed using STN Express query preparation: Uploading L9L10.str

chain nodes :

19 20 21 22 29 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27

chain bonds :

13-21 16-22 19-21 20-22 21-32 22-25

ring bonds :

exact/norm bonds :

5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-22 21-32 22-25

normalized bonds :

25-26 26-27 27-28

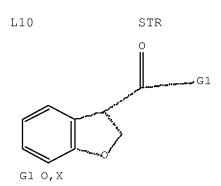
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Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:CLASS

22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS 32:CLASS

fragments assigned product role: containing 7 fragments assigned reactant/reagent role: containing 1 node mappings: 14:17 13:16



Structure attributes must be viewed using STN Express query preparation.

L12	1802 SEA FILE=REGISTRY SUB=L5 SSS FUL L9	
L14	7056 SEA FILE=REGISTRY SUB=L5 SSS FUL L10	
L17	230 SEA FILE=CAPLUS ABB=ON PLU=ON L12 (L) PREP/RL	
L18	312 SEA FILE=CAPLUS ABB=ON PLU=ON L14 (L) (RACT OR RGT OR	
	RCT)/RL	
L19	5 SEA FILE=CAPLUS ABB=ON PLU=ON L17 AND L18	
L21	4 SEA FILE=CAPLUS ABB=ON PLU=ON BLEGER F?/AU	
L22	2 SEA FILE=CAPLUS ABB=ON PLU=ON MORDACQ F?/AU	
L23	66 SEA FILE=CAPLUS ABB=ON PLU=ON PIRON J?/AU	
L26	37 SEA FILE=CAPLUS ABB=ON PLU=ON SCHOUTEETEN A?/AU	
L31	1 SEA FILE=CAPLUS ABB=ON PLU=ON L19 AND (L21 OR L22 OR L23 O	R
	L26)	

=> s L30 or L31 L36 3 L30 OR L31

=> file casreact

FILE 'CASREACT' ENTERED AT 10:46:02 ON 19 FEB 2008 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE CONTENT: 1840 - 16 Feb 2008 VOL 148 ISS 8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

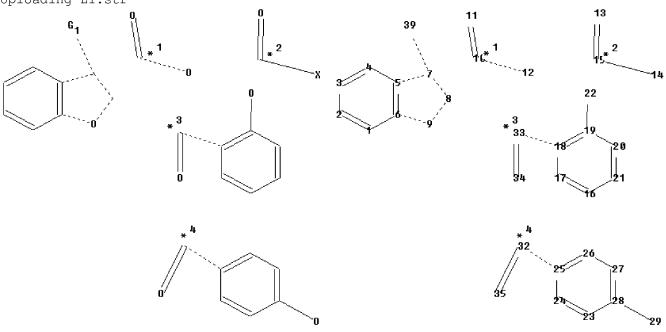
Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L35 L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation: Uploading L1.str



chain nodes : 10 11 12 13 14 15 22 29 32 33 34 35 39 ring nodes : 1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 chain bonds : $7-39 \quad 10-12 \quad 10-11 \quad 13-15 \quad 14-15 \quad 18-33 \quad 19-22 \quad 25-32 \quad 28-29 \quad 32-35 \quad 33-34$ ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20$ 20-21 23-24 23-28 24-25 25-26 26-27 27-28 exact/norm bonds : 5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-35 33 - 34exact bonds : 14 - 15normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21 \quad 23-24 \quad 23-19 \quad$ 28 24-25 25-26 26-27 27-28

G1:[*1],[*2],[*3],[*4]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom

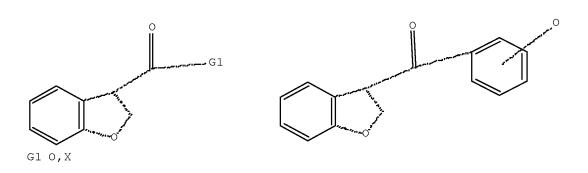
19:Atom 20:Atom 21:Atom

22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS

33:CLASS

34:CLASS 35:CLASS 39:CLASS

L3 STR



Structure attributes must be viewed using STN Express query preparation:

Uploading L3.str

chain nodes :

19 20 21 22 29 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27

chain bonds :

13-21 16-22 19-21 20-22 21-32 22-25

ring bonds :

exact/norm bonds :

5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-22 21-32 22-25

normalized bonds :

25-26 26-27 27-28

G1:0,X

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

20:CLASS 21:CLASS

22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS

32:CLASS

fragments assigned product role:

containing 7

fragments assigned reactant/reagent role:

containing 1
node mappings:
14:17 13:16

L5 8858 SEA FILE=REGISTRY SSS FUL L1 L6 324 SEA FILE=CASREACT ABB=ON PLU=ON L5

L8 2 SEA FILE=CASREACT SUB=L6 SSS FUL L3 (8 REACTIONS)

L34 1 SEA FILE=CASREACT ABB=ON PLU=ON ("143:97254"/AN OR "2005:5690

50"/AN)

L35 1 SEA FILE=CASREACT ABB=ON PLU=ON L34 AND L8

=> d ibib abs hitstr L36 1-3; d ibib abs hit L35 1
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L36 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:569050 CAPLUS Full-text

DOCUMENT NUMBER: 143:97254

TITLE: Process for preparation de 2-(n-alky1)-3-(4-alky1)

hydroxybenzoyl)benzofurans and intermediates by halogenation of carboxybenzofuran derivatives, Friedel-Crafts acylation with alkoxybenzenes and

dealkylation

INVENTOR(S): Schouteeten, Alain; Bleger, Francois; Mordacq,

Françoise; Piron, Jerome

PATENT ASSIGNEE(S): Clariant France, Fr. SOURCE: Fr. Demande, 22 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO	KIN	D :	DATE			APPL	ICAT	DATE							
FR 286453								8		2	0031	224			
FR 286453 WO 200506	B1 A1		2006 2005		WO 2004-IB4158						20041215				
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С	N, CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
G	E, GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,
L	K, LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,

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NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
            MR, NE, SN, TD, TG
     EP 1699772
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                                           EP 2004-801395
                                                                   20041215
                         A 1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS
     CN 1898226
                                20070117
                                           CN 2004-80038285
                         Α
                                                                   20041215
     JP 2007517012
                          Τ
                                20070628
                                           JP 2006-546365
                                                                   20041215
     NO 2006002936
                         Α
                                20060922
                                           NO 2006-2936
                                                                   20060623
     IN 2006CN02324
                         Α
                                20070706
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                                                                   20060626
     US 2007155831
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                                                                   20061129
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PRIORITY APPLN. INFO.:
                                            FR 2003-15398
                                                                A 20031224
                                            WO 2004-IB4158
                                                              W 20041215
OTHER SOURCE(S):
                       CASREACT 143:97254
GΙ
```

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

The invention is related to the preparation of benzofurans I [R = linear or]AΒ branched alkyl; R1 = halo, NO2, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C6H5OR2 (III) [R2 = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R1, R2 defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO2; R4 = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5- nitrobenzofuran with SOCl2 in PhCl, acylation of anisole with acyl chloride in the presence of AlCl3, and demethylation over AlC13 at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO2, R = n-Bu] after purification Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)-benzofuran in the presence of acetic anhydride/H2SO4 for 2 h gave acid II (m.p. = 207°). 141627-42-1P, 2-(n-Butyl)-3-(4-methoxybenzoyl)-5-nitrobenzofuranΙT 856758-02-6P, 2-(n-Butyl)-3-carboxy-5-nitrobenzofuran 856758-03-7P, 2-(n-Butyl)-3-chlorocarbonyl-5-nitrobenzofuran 856758-04-8P, 2-(n-Buty1)-3-(2-methoxybenzoy1)-5-nitrobenzofuranRL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or (intermediate; process for preparation de 2-(n-alkyl)-3-(4hydroxybenzoyl) benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)

$$O_2N \longrightarrow O_1 \longrightarrow O_2N \longrightarrow O_2N \longrightarrow O_3 \longrightarrow O$$

RN 856758-02-6 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-butyl-5-nitro- (CA INDEX NAME)

856758-03-7 CAPLUS RN

CN 3-Benzofurancarbonyl chloride, 2-butyl-5-nitro- (CA INDEX NAME)

$$O_2N \longrightarrow O_2N$$

$$Bu-n$$

RN 856758-04-8 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(2-methoxyphenyl)- (CA INDEX NAME)

856758-05-9P, 2-(n-Buty1)-3-(2-hydroxybenzoy1)-5-nitrobenzofuranΙT

RL: BYP (Byproduct); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl) benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans,

Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

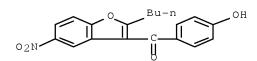
RN 856758-05-9 CAPLUS

Methanone, (2-butyl-5-nitro-3-benzofuranyl)(2-hydroxyphenyl)- (CA INDEX CN NAME)

IT 141645-16-1P, 2-(n-Butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(product; process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

- RN 141645-16-1 CAPLUS
- CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L36 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:1018469 CAPLUS Full-text

DOCUMENT NUMBER: 141:425581

TITLE: Process for separating glyoxal diacetals from crude mixtures by countercurrent liquid-liquid extraction

INVENTOR(S): Simon, Olivier; Bleger, François; Schouteeten, Alain

PATENT ASSIGNEE(S): ClariantFrance, Fr. SOURCE: Fr. Demande, 22 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE					APPLICATION NO.						DATE			
FR 2855171				A1 20041126					FR 2003-6168						20030522			
FR 2855171 WO 2004106274				B1 20050805 A1 20041209			,	WO 2004-FR1224						20040518				
W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
	GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,		
	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,		
	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW		
RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
	ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	ΙT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,		

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10/584440
                SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
                SN, TD, TG
                               A1 20060215 EP 2004-742769
           R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
      CN 1795157 A 20060628 CN 2004-80014034

JP 2007502318 T 20070208 JP 2006-530363

US 2007073088 A1 20070329 US 2005-557920

IN 2005CN03483 A 20070914 IN 2005-CN3483
                                                                                 20040518
                                                                                 20051122
                                                                                 20051222
PRIORITY APPLN. INFO.:
                                                     FR 2003-6168
                                                                             A 20030522
                                                     WO 2004-FR1224 W 20040518
       (RO) 2CHCH(OR)2 (R = C1-4 \text{ alkyl}) is separated from acetalization product mixts.
AΒ
       also containing (RO) 2CHCHO (R = C1-4 alkyl) by discontinuous or continuous
       countercurrent liquid-liquid extraction using solvents not miscible with the
       reaction media.
                               5
REFERENCE COUNT:
                                      THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
                                      RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT
L36 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:524688 CAPLUS <u>Full-text</u>
DOCUMENT NUMBER:
                              135:92535
TITLE:
                             Process for the preparation of 3-(1-
                             hydroxypentylidene)-5-nitro-3H-benzofuran-2-one and
                              its ketone tautomeric form 3-(1-oxo-pentyl)-5-nitro-3H-
                             benzofuran-2-one
INVENTOR(S):
                              Schouteeten, Alain; Mordacq, Françoise
                         Clariant (France) S.A., Fr.
PATENT ASSIGNEE(S):
SOURCE:
                              Eur. Pat. Appl., 5 pp.
                              CODEN: EPXXDW
DOCUMENT TYPE:
                              Patent
LANGUAGE:
                              English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
      PATENT NO. KIND DATE APPLICATION NO. DATE
      PATENT NO.
                                                                                  ______
      EP 1116719
                             A2 20010718 EP 2001-810033
                                                                                20010115
      EP 1116719 A3 20011024
EP 1116719 B1 20050406
           R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                IE, SI, LT, LV, FI, RO
      FR 2803846 A1 20010720 FR 2000-523
                                                                                   20000117
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TW 564246
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B 20031201
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20010117
US 2001012900
A1 20010809
US 2001-761452
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US 6515147
B2 20030204
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IN 2003-MA433
20030528
US 39755
E1 20070731
US 2001-761452
E 20010117
                              В1
                                      20020405
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CASREACT 135:92535 OTHER SOURCE(S):

PRIORITY APPLN. INFO.:

US 2001-761452 E 20010117

AB 3-(1-Hydroxypentylidene)-5-nitro-3H-benzofuran-2-one, and to its ketone tautomeric form 3-(1-oxo-pentyl)-5-nitro-3H-benzofuran-2-one, are prepared in

high yield and selectivity by the reaction of 5-nitro-3H-benzofuran-2- one at $>30^{\circ}$ with pentanoic anhydride and a salt of pentanoic acid, optionally in the presence of pentanoic acid, then the resulting reaction mixture is acidified (e.g., sulfuric acid) and the precipitated product (m.p. 164°, DSC) collected by filtration.

```
L35 ANSWER 1 OF 1 CASREACT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 143:97254 CASREACT Full-text
```

TITLE:

Process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of carboxybenzofuran derivatives, Friedel-Crafts acylation with alkoxybenzenes and

dealkylation

INVENTOR(S): Schouteeten, Alain; Bleger, Francois; Mordacq,

Francoise; Piron, Jerome

PATENT ASSIGNEE(S): Clariant France, Fr. SOURCE: Fr. Demande, 22 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO. K.					KIND DATE					APPLICATION NO.					DATE			
		2864 2864					2005 2006								2003	1224			
		2005			_	_				TAT	0 20	∩4-т	R415	8	2004	1215			
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		RW.	•	,	,	•	,	,	,	,	,	,	,	•	UG,	•	,		
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	CN	1898	,	,	,	,	,	,	,	,	,	,	,	,	2004				
	JР	2007	5170	12	Т		2007	0628		J	P 20	06-5	4636	5	2004	1215			
		2006													2006				
										IN 2006-CN2324									
	US	2007	1558	31	А	1	2007	0705		US 2006-584440									
PRIO	RIT	Y APP	LN.	INFO	.:					F	R 20	03-1	5398		2003	1224			
															2004				

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AΒ The invention is related to the preparation of benzofurans I [R = linear or]branched alkyl; R1 = halo, NO2, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C6H5OR2 (III) [R2 = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R1, R2 defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO2; R4 = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5- nitrobenzofuran with SOC12 in PhCl, acylation of anisole with acyl chloride in the presence of AlCl3, and demethylation over AlC13 at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO2, R = n-Bu] after purification Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)-benzofuran in the presence of acetic anhydride/H2SO4 for 2 h gave acid II (m.p. = 207°). REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 14 ...2 E + 2 B ===> F + G...

$$E$$
 $O2N$
 $Bu-n$
 $C1$
 E
 $O2N$
 $C2$
 $C2$

RX(2)

STAGE(1)

RGT H 7446-70-0 AlC13

SOL 108-90-7 PhC1

CON room temperature -> 0 deg C

STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

STAGE(3)

RCT B 856758-03-7

CON SUBSTAGE(1) 1 hour, 5 deg C

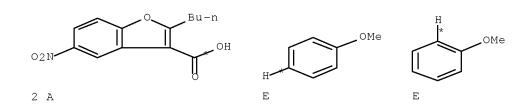
SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C

SUBSTAGE(3) 3 hours, room temperature

PRO F 141627-42-1, G 856758-04-8

NTE Friedel-Crafts reaction, regioselective(4-methoxy product is the major isomer)





RX(7) 2 E + 2 B ===> I

```
RX(1)
       RCT A 856758-02-6
           STAGE(1)
              SOL 108-90-7 PhCl
              CON room temperature -> 80 deg C
           STAGE(2)
              RGT C 7719-09-7 SOC12
              CON SUBSTAGE(1) 20 minutes, 80 deg C
                   SUBSTAGE(2) 9 hours, 80 deg C
         PRO B 856758-03-7
         NTE anisole alternately used as solvent
RX(2)
           STAGE(1)
              RGT H 7446-70-0 AlC13
              SOL 108-90-7 PhCl
              CON room temperature -> 0 deg C
           STAGE(2)
              RCT E 100-66-3
              CON 15 minutes, 0 deg C
           STAGE (3)
              RCT B 856758-03-7
              CON SUBSTAGE(1) 1 hour, 5 deg C
                   SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C
                   SUBSTAGE(3) 3 hours, room temperature
         PRO F 141627-42-1, G 856758-04-8
         NTE Friedel-Crafts reaction, regioselective (4-methoxy product is the
              major isomer)
RX(7) OF 14 COMPOSED OF RX(2), RX(3)
```

Ι

RX(2)

```
STAGE(1)
               RGT H 7446-70-0 AlC13
               SOL 108-90-7 PhCl
               CON room temperature -> 0 deg C
            STAGE(2)
               RCT E 100-66-3
               CON 15 minutes, 0 deg C
            STAGE(3)
               RCT B 856758-03-7
               CON SUBSTAGE(1) 1 hour, 5 deg C
                    SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C
                    SUBSTAGE(3) 3 hours, room temperature
          PRO F 141627-42-1, G 856758-04-8
          NTE Friedel-Crafts reaction, regioselective (4-methoxy product is the
               major isomer)
RX(3)
         RCT F 141627-42-1
            STAGE (1)
```

RGT H 7446-70-0 AlC13 SOL 108-90-7 PhC1

CON 7 hours, room temperature -> 60 deg C

STAGE(2)

RGT J 7732-18-5 Water

PRO I 141645-16-1

 ${\tt RX(8)}$ OF 14 COMPOSED OF ${\tt RX(2)}$, ${\tt RX(5)}$

RX(8) 2 E + 2 B ===> I + N

STEPS

$$O_2N$$

$$M$$

$$O_2N$$

$$M$$

$$N$$

$$N$$

RX(2)

STAGE(1)

RGT H 7446-70-0 AlC13

SOL 108-90-7 PhCl

CON room temperature -> 0 deg C

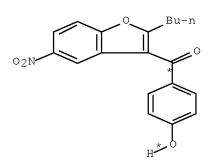
STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

STAGE(3) RCT B 856758-03-7 CON SUBSTAGE(1) 1 hour, 5 deg C SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C SUBSTAGE(3) 3 hours, room temperature PRO F 141627-42-1, G 856758-04-8 NTE Friedel-Crafts reaction, regioselective (4-methoxy product is the major isomer) RX(5) RCT F 141627-42-1, G 856758-04-8 STAGE (1) RGT H 7446-70-0 AlC13 SOL 108-90-7 PhCl CON 7 hours, room temperature -> 60 deg C STAGE(2) RGT J 7732-18-5 Water CON 60 deg C PRO I 141645-16-1, N 856758-05-9 RX(10) OF 14 COMPOSED OF RX(1), RX(2), RX(3)RX(10) 2 A + 2 E ===> I Bu-n оме Ε 2 A

3 STEPS



Ι

```
RCT A 856758-02-6
RX(1)
           STAGE(1)
              SOL 108-90-7 PhCl
              CON room temperature -> 80 deg C
           STAGE(2)
              RGT C 7719-09-7 SOC12
              CON SUBSTAGE(1) 20 minutes, 80 deg C
                   SUBSTAGE(2) 9 hours, 80 deg C
         PRO B 856758-03-7
         NTE anisole alternately used as solvent
RX(2)
           STAGE(1)
              RGT H 7446-70-0 AlC13
              SOL 108-90-7 PhCl
              CON room temperature -> 0 deg C
           STAGE(2)
              RCT E 100-66-3
              CON 15 minutes, 0 deg C
           STAGE(3)
              RCT B 856758-03-7
              CON SUBSTAGE(1) 1 hour, 5 deg C
                   SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C
                   SUBSTAGE(3) 3 hours, room temperature
         PRO F 141627-42-1, G 856758-04-8
         NTE Friedel-Crafts reaction, regioselective (4-methoxy product is the
              major isomer)
         RCT F 141627-42-1
RX(3)
           STAGE (1)
              RGT H 7446-70-0 AlC13
              SOL 108-90-7 PhCl
              CON 7 hours, room temperature -> 60 deg C
           STAGE (2)
              RGT J 7732-18-5 Water
         PRO I 141645-16-1
RX(11) OF 14 COMPOSED OF RX(1), RX(2), RX(5)
RX(11) 2 A + 2 E ===> I + N
```

STEPS

STAGE(1)

SOL 108-90-7 PhC1

CON room temperature -> 80 deg C

STAGE(2)

RGT C 7719-09-7 SOC12

CON SUBSTAGE(1) 20 minutes, 80 deg C

SUBSTAGE(2) 9 hours, 80 deg C

RCT A 856758-02-6

PRO B 856758-03-7 NTE anisole alternately used as solvent

RX(2)

RX(1)

STAGE(1)

RGT H 7446-70-0 AlC13

SOL 108-90-7 PhC1

CON room temperature -> 0 deg C

STAGE(2)

RCT E 100-66-3

CON 15 minutes, 0 deg C

```
STAGE(3)
              RCT B 856758-03-7
              CON SUBSTAGE(1) 1 hour, 5 deg C
                   SUBSTAGE(2) 1 hour, 5 deg C -> 20 deg C
                   SUBSTAGE(3) 3 hours, room temperature
         PRO F 141627-42-1, G 856758-04-8
         NTE Friedel-Crafts reaction, regioselective (4-methoxy product is the
              major isomer)
RX(5)
         RCT F 141627-42-1, G 856758-04-8
           STAGE(1)
              RGT H 7446-70-0 AlC13
              SOL 108-90-7 PhCl
              CON 7 hours, room temperature -> 60 deg C
           STAGE(2)
              RGT J 7732-18-5 Water
              CON 60 deg C
         PRO I 141645-16-1, N 856758-05-9
ΑN
   143:97254 CASREACT Full-text
```

=> file registry
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FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8 FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

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'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L19 L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation:

Uploading L1.str

61

22

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chain nodes : 10 11 12 13 14 15 22 29 32 33 34 35 39 ring nodes : 1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 28 chain bonds : 7-39 10-12 10-11 13-15 14-15 18-33 19-22 25-32 28-29 32-35 33-34 ring bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-7 \quad 6-9 \quad 7-8 \quad 8-9 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20$ 20-21 23-24 23-28 24-25 25-26 26-27 27-28 exact/norm bonds : 5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-3533-34 exact bonds : 14 - 15normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21 \quad 23-24 \quad 23-19 \quad$ 24-25 25-26 26-27 27-28

G1:[*1],[*2],[*3],[*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS 33:CLASS 35:CLASS 39:CLASS

L5 8858 SEA FILE=REGISTRY SSS FUL L1 L9 STR

Structure attributes must be viewed using STN Express query preparation: Uploading L9L10.str

chain nodes :

19 20 21 22 29 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27 28

chain bonds :

13-21 16-22 19-21 20-22 21-32 22-25

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 5-13 \quad 6-15 \quad 7-8 \quad 7-12 \quad 8-9 \quad 9-10 \quad 10-11 \quad 11-12 \quad 11-16$ $12 - 18 \quad 13 - 14 \quad 14 - 15 \quad 16 - 17 \quad 17 - 18 \quad 23 - 24 \quad 23 - 28 \quad 24 - 25 \quad 25 - 26 \quad 26 - 27 \quad 27 - 28$

exact/norm bonds :

5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-2221-32 22-25

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-12 \quad 8-9 \quad 9-10 \quad 10-11 \quad 11-12 \quad 23-24 \quad 23-28 \quad 24-129 \quad 23-24 \quad 23-2$

25

25-26 26-27 27-28

G1:0,X

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

20:CLASS 21:CLASS

22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS

32:CLASS

fragments assigned product role:

containing 7

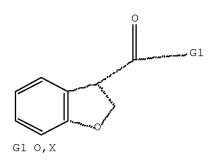
fragments assigned reactant/reagent role:

containing 1

node mappings:

14:17 13:16

L10 STR



Structure attributes must be viewed using STN Express query preparation.

L12	1802	SEA FILE=REGIST	RY SUB=L5	SSS FUI	L L9		
L14	7056	SEA FILE=REGIST	RY SUB=L5	SSS FUI	L L10		
L17	230	SEA FILE=CAPLUS	ABB=ON	PLU=ON	L12 (L)	PREP/RL	
L18	312	SEA FILE=CAPLUS	ABB=ON	PLU=ON	L14 (L)	(RACT OR	RGT OR
		RCT)/RL					
L19	5	SEA FILE=CAPLUS	ABB=ON	PLU=ON	L17 AND	L18	

=> s L19 not L36

L37 4 L19 NOT L36

=> file casreact

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FILE CONTENT:1840 - 16 Feb 2008 VOL 148 ISS 8

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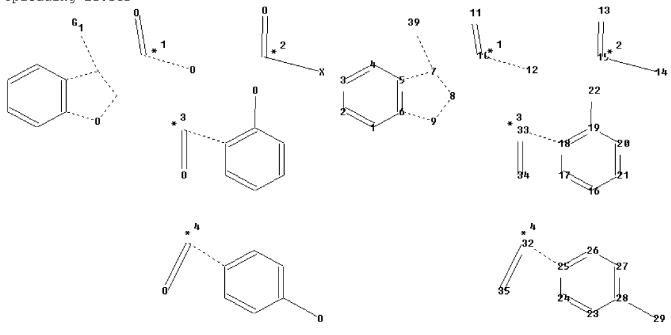
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=> d stat que L8 L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation: Uploading L1.str



chain nodes : 10 11 12 13 14 15 22 29 32 33 34 35 39 ring nodes : 1 2 3 4 5 6 7 8 9 16 17 18 19 20 21 23 24 25 26 27 28 chain bonds : 7-39 10-12 10-11 13-15 14-15 18-33 19-22 25-32 28-29 32-35 33-34ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9 16-17 16-21 17-18 18-19 19-2020-21 23-24 23-28 24-25 25-26 26-27 27-28 exact/norm bonds : 5-7 6-9 7-8 7-39 8-9 10-12 10-11 13-15 18-33 19-22 25-32 28-29 32-3533 - 34exact bonds : 14 - 15normalized bonds : $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 16-17 \quad 16-21 \quad 17-18 \quad 18-19 \quad 19-20 \quad 20-21 \quad 23-24 \quad 23-19 \quad$ 24-25 25-26 26-27 27-28

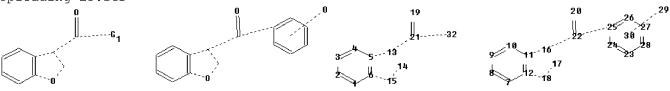
G1:[*1],[*2],[*3],[*4]

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom 18:Atom
19:Atom 20:Atom 21:Atom
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 32:CLASS
33:CLASS 33:CLASS 39:CLASS 39:CLASS

L3 STR

$$\bigcap_{G1 \text{ O, X}} \bigcap_{G1} \bigcap_{G1$$

Structure attributes must be viewed using STN Express query preparation: Uploading L3.str



chain nodes :

19 20 21 22 29 32

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 23 24 25 26 27 28

chain bonds :

13-21 16-22 19-21 20-22 21-32 22-25

ring bonds :

exact/norm bonds :

5-13 6-15 11-16 12-18 13-14 13-21 14-15 16-17 16-22 17-18 19-21 20-22

21-32 22-25

normalized bonds :

25-26 26-27 27-28

G1:0,X

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS
20:CLASS 21:CLASS
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
fragments assigned product role:
containing 7
fragments assigned reactant/reagent role:
containing 1
node mappings:
14:17 13:16

L5 8858 SEA FILE=REGISTRY SSS FUL L1

L6 324 SEA FILE=CASREACT ABB=ON PLU=ON L5

L8 2 SEA FILE=CASREACT SUB=L6 SSS FUL L3 (8 REACTIONS)

100.0% DONE 254 VERIFIED 8 HIT RXNS 2 DOCS

SEARCH TIME: 00.00.01

=> s 18 not L35

L38 1 L8 NOT L35

=> dup rem L38 L37

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PROCESSING COMPLETED FOR L38 PROCESSING COMPLETED FOR L37

L39 5 DUP REM L38 L37 (0 DUPLICATES REMOVED)

ANSWER '1' FROM FILE CASREACT ANSWERS '2-5' FROM FILE CAPLUS

=> d ibib abs hit L39 1; d ibib abs hitind hitstr L39 2-5

L39 ANSWER 1 OF 5 CASREACT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 108:21130 CASREACT Full-text

TITLE: Conformational analysis of organic carbonyl compounds.

Part 5. p-Methoxybenzoyl derivatives of

benzo[b]furan, benzo[b]thiophene, and naphthalene

AUTHOR(S): Benassi, Rois; Folli, Ugo; Larossi, Dario; Schenetti,

Luisa; Taddei, Ferdinando

CORPORATE SOURCE: Dip. Chim., Univ. Modena, Modena, 41100, Italy

SOURCE: Journal of the Chemical Society, Perkin Transactions

2: Physical Organic Chemistry (1972-1999) (1987),

(3), 351-7

CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal LANGUAGE: English

AB The conformational anal. of 2- and 3-(p-methoxybenzoyl)benzo[b]furan and -benzo[b]thiophene and 1- and 2-(p-methoxybenzoyl)naphthalene was performed by the NMR lanthanide-induced shift method on 1H and 13C chemical shifts with Yb(fod)3. In the 2-substituted benzo[b]furan a chelate structure having the lanthanide atom bound to both carbonyl and furyl oxygens is formed, so the results do not represent useful information for the conformational properties of the mol. in solution For the 2-benzo[b]thiophene derivative the S,O-cis (Z) conformation was found to be more abundant in the equilibrium mixture of the two nearly planar conformers. In the corresponding 3-substituted heterocycles the predominant conformation is that of X,O-trans type with a similar degree of distortion from planarity in the two compds. In all these mols. the p-methoxyphenyl ring is twisted .apprx.30° from the carbonyl plane.

$$RX(2)$$
 OF 4 ...D + B ===> \mathbb{H}

$$_{\rm D}^{\rm OMe}$$
 $_{\rm C1}^{\rm C1}$ $_{\rm B}$

E YIELD 44%

$$RX(4)$$
 OF 4 COMPOSED OF $RX(1)$, $RX(2)$ $RX(4)$ A + D ===> E

E YIELD 44%

RX(1) RCT A 26537-68-8 RGT C 7719-09-7 SOC12 PRO B 111964-21-7 SOL 7719-09-7 SOC12 RX(2) RCT D 100-66-3, B 111964-21-7 RGT F 7446-70-0 AlC13 PRO E 28222-80-2 SOL 75-15-0 CS2

L39 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:99174 CAPLUS $\underline{\text{Full-text}}$

DOCUMENT NUMBER: 142:198073

TITLE: Preparation of heterocyclic compounds useful as

malonyl-CoA decarboxylase inhibitors

INVENTOR(S): Cheng, Jie Fei; Nguyen, Bao Ngoc; Liu, Xuewei;

Lopaschuk, Gary D.; Dyck, Jason R.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 18 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	PATENT NO.			KIND DATE			APPLICATION NO.											
US	2005	0269	69						US 2004-900958									
CA	2533	747			A1 20050210			CA 2004-2533747						20040728				
WO	2005	0116	70		A1		2005	0210		WO 2	004-	US24	285		20040728			
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	ВG,	BR,	BW,	BY,	BZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LC,	
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	
		ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	
		AZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,	
		SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GO,	GW,	ML,	MR,	NE,	
		•	TD,		·	·	·	·	·	·	ŕ	,	~,	·	,	·	,	
EP	1653	944	·		A1 20060510				EP 2004-757346					20040728				
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		•	•				•	MK,		•						•		HF
JP	2007																	
CIORIT										US 2								
										WO 2		-						
HER SO	OURCE	(S):			CASI	REAC	T 14	2:19							. .			

The present invention provides methods for the use of compds. I [X1, X2, X3]AΒ O, N, NH, NR5, S, C; R1, R2 = H, halogen, substituted C1-6-alkyl, substituted C1-6-alkenyl, substituted C1-6-alkynyl, alkoxy, (un)substituted Ph, aryl, (un) substituted heteroaryl, NHCONR5R6, COR5, CONR5R6, S(O)nR5, SO2NR5R6; R3, R4 = H, Br, C1, F, I, OH, OMe, CO2H, CO2R5, CONR5R6, S(O)nR5, SO2NR5R6, substituted C1-6-alkyl, C1-6-alkoxy, (un) substituted Ph, aryl, heteroaryl; R5, R6 = H, (un)substituted C1-6-alkyl, (un)substituted Ph, aryl, heteroaryl], its enantiomers, diastereomers, tautomers, or physiol. acceptable salts or prodrugs, pharmaceutical compns. containing the same, and methods for the prophylaxis, management and treatment of metabolic diseases and diseases modulated by MCD inhibition. Thus, benzofuran I [X1 = CC(:0)NHC6H3(OMe)2-3,4, X2 = CH, X3 = O, R3 = 4-Br, R4 = 6-Br] was prepared from 5-methoxybenzofuran-2- carboxylic acid via regioselective bromination at C(3), decarboxylation, debromination-carboxylation at C(3), O-demethylation, regioselective dibromination and amidation with 3,4-dimethoxyaniline. The compds. disclosed in this invention are useful for the prophylaxis, management and treatment of diseases involving in malonyl-CoA regulated glucose/fatty acid metabolism pathway. The inhibitory activity of I vs. malonyl-CoA decarboxylase was determined [Ki = $31.6 - 4750.2 \mu M$]. In particular, these compds. and pharmaceutical composition containing the same are indicated in the prophylaxis, management and treatment of cardiovascular diseases, diabetes, cancer and obesity.

IC ICM A61K031-433

as

as

ICS A61K031-428; A61K031-4245; A61K031-423; A61K031-4184

INCL 514363000; 514364000; 514367000; 514375000; 514394000

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7, 27, 63

IT 23455-49-4P 383159-30-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and O-demethylation of; preparation of heterocyclic compds. useful

as malonyl-CoA decarboxylase inhibitors)

IT 836629-05-1P, 4,6-Dibromo-5-hydroxybenzofuran-2-carboxylic acid 836629-06-2P, 4,6-Dibromo-5-hydroxybenzofuran-3-carboxylic acid

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and amidation of; preparation of heterocyclic compds. useful

malonyl-CoA decarboxylase inhibitors)

IT 29735-85-1P, 5-Hydroxybenzofuran-3-carboxylic acid 56172-36-2P,

5-Hydroxybenzofuran-2-carboxylic acid 251477-67-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

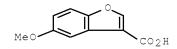
(Preparation); RACT (Reactant or reagent)

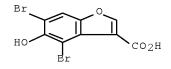
(preparation and bromination of; preparation of heterocyclic compds. useful

malonyl-CoA decarboxylase inhibitors)

IT 41967-46-8P 41967-47-9P 412966-58-6P 836628-69-4P,

```
2-Benzoyl-4,6-dibromo-5-hydroxybenzofuran
                                                 836628-70-7P
                                                                 836628-71-8P
     836628-72-9P
                   836628-73-0P
                                   836628-74-1P
                                                 836628-75-2P
                                                                 836628-76-3P
     836628-78-5P
                    836628-79-6P
                                   836628-80-9P
                                                  836628-81-0P
                                                                  836628-82-1P
     836628-83-2P
                    836628-84-3P
                                   836628-85-4P
                                                  836628-86-5P
                                                                  836628-87-6P
     836628-88-7P
                    836628-89-8P
                                   836628-90-1P
                                                  836628-91-2P
                                                                  836628-92-3P
     836628-93-4P
                    836628-94-5P
                                   836628-95-6P
                                                  836628-96-7P
                                                                  836628-97-8P
     836628-98-9P
                    836628-99-0P
                                   836629-00-6P
                                                  836629-01-7P
                                                                 836629-02-8P
     836629-03-9P
                    836629-04-0P
                                   836629-38-0P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation);
     USES (Uses)
        (preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase
        inhibitors)
ΙT
     23455-49-4P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (preparation and O-demethylation of; preparation of heterocyclic compds.
useful
        as malonyl-CoA decarboxylase inhibitors)
RN
     23455-49-4 CAPLUS
CN
     3-Benzofurancarboxylic acid, 5-methoxy- (CA INDEX NAME)
```





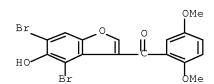
IT 412966-58-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic compds. useful as malonyl-CoA decarboxylase inhibitors)

RN 412966-58-6 CAPLUS

CN Methanone, (4,6-dibromo-5-hydroxy-3-benzofuranyl)(2,5-dimethoxyphenyl)- (CA INDEX NAME)



L39 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1997:8073 CAPLUS Full-text

DOCUMENT NUMBER: 126:144080

TITLE: β -(2-Benzofuranyl)enamines and

(2-indoly1)enamines in the Nenitzescu reaction

AUTHOR(S): Mukhanova, Tatyana I.; Panisheva, Elena K.;

Lyubchanskaya, Valeriya M.; Alekseeva, Lyudmila M.;

Sheinker, Yurvi N.; Granik, Vladimir G.

CORPORATE SOURCE: Center for Drug Chemistry, All Russian Res.

Chemical-Pharmaceutical Institute, Moscow, Russia

SOURCE: Tetrahedron (1997), 53(1), 177-184

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Depending on the volume and electron-withdrawing properties of the substituents in the heterocyclic ring, reaction of β -(2-benzofuranyl)- and (2-indolyl)enamines with benzoquinone led to the formation of 3-heteroarylbenzofurans, with or without a dimethylamino group in the position

2. If dehydrogenation was impossible, as in the case of α -methyl- β -

heteroarylenamines, furo[2,3-f]benzofurans are formed.

CC 27-11 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 25

IT 128944-24-1P 163890-14-0P 186553-66-2P 186553-75-3P

186553-76-4P 186553-79-7P 186553-80-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)

IT 186553-67-3P 186553-68-4P 186553-70-8P 186553-71-9P

186553-72-0P 186553-73-1P 186553-74-2P 186553-77-5P

186553-78-6P 186553-81-1P 186553-82-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)

IT 186553-66-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

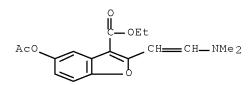
(Preparation); RACT (Reactant or reagent)

(Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)

RN 186553-66-2 CAPLUS

 ${\tt CN} \qquad {\tt 3-Benzofurancarboxylic\ acid,\ 5-(acetyloxy)-2-[2-(dimethylamino)ethenyl]-,}$

ethyl ester (CA INDEX NAME)



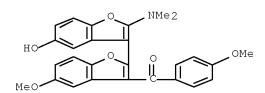
IT 186553-72-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(Nenitzescu reaction of (aminovinyl)indoles or (aminovinyl)benzofurans)

RN 186553-72-0 CAPLUS

CN Methanone, [2'-(dimethylamino)-5'-hydroxy-5-methoxy[2,3'-bibenzofuran]-3-yl](4-methoxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L39 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1974:403757 CAPLUS Full-text

DOCUMENT NUMBER: 81:3757
ORIGINAL REFERENCE NO.: 81:607a,610a

TITLE: Antiangina benzofuran derivatives

INVENTOR(S): Descamps, Marcel; Gubin, Jean; Claeys, Norbert

PATENT ASSIGNEE(S): Labaz

SOURCE: Ger. Offen., 38 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2347196	A1	19740328	DE 1973-2347196	19730919
ZA 7305652	A	19741030	ZA 1973-5652	19730817

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AU 7359650
                      Α
                               19750227
                                          AU 1973-59650
                                                                 19730827
    FI 55336
                       С
                               19790710
                                         FI 1973-2715
                                                                 19730831
    FI 55336
                       В
                               19790330
    CA 983502
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                               19760210
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                                                                 19730904
                                           BE 1973-135394
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    US 3920707
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                               19751118
                                          US 1973-395847
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    GB 1382742
                        Α
                               19750205
                                          GB 1972-43387
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                               19760915
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    NL 7312817
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    DK 133899
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                               19780823
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    AT 325034
                         В
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                               19760301
                                          ES 1973-418892
                                                                 19730919
                                           GB 1972-43387
PRIORITY APPLN. INFO.:
                                                             A 19720919
    For diagram(s), see printed CA Issue.
    Benzofurans I (R = C1-4 alkyl, cyclohexyl; R1 = H, Me, Et, Pr; NR2R3 = NH2,
AΒ
     alkylamino, dialkylamino, heterocyclic amino; n = 3-6) (70 compds.) were
     prepared Thus I (R = Et, R1 = Me, NR2R3 = NBu2, n = 3) (II) was prepared by
     converting 2-ethyl-3-benzofurancarboxylic acid to its chloride, treating with
     2,6-Me2C6H3OMe, ether cleavage of the 2-ethyl-3-(3,5- dimethyl-4-
     methoxybenzoyl)benzofuran, treating the hydroxy compound with Br(CH2)3Br and
     Bu2NH. II was as active as 2-buty1-3-(3,5-diiodo-4-y-
     dimethylaminopropoxybenzoyl)benzofuran in reducing the heart rate of
     anesthetized dogs.
IC
    C07D; A61K
CC
    27-7 (Heterocyclic Compounds (One Hetero Atom))
ΙT
    52489-45-9P 52489-46-0P 52489-47-1P
    52489-48-2P 52489-49-3P 52489-50-6P
    52489-51-7P 52489-52-8P 52489-53-9P
    52489-54-0P 52489-55-1P 52489-56-2P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and ether cleavage of)
ΙT
    52489-70-0P 52489-71-1P 52489-72-2P
    52489-73-3P 52489-74-4P 52490-16-1P
    52490-52-5P 52490-53-6P 52490-61-6P
    52490-62-7P 52490-69-4P 52490-70-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP
    (Preparation); RACT (Reactant or reagent)
        (preparation and reaction of, with amines)
    52489-35-7P 52489-36-8P 52489-37-9P
ΙT
    52489-38-0P 52489-39-1P 52489-40-4P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (preparation and reaction of, with dialkylanisoles)
ΙT
    52489-58-4P 52489-59-5P 52489-60-8P
    52489-61-9P 52489-62-0P 52489-63-1P
    52489-64-2P 52489-65-3P 52489-66-4P
    52489-67-5P 52489-68-6P 52489-69-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (preparation and reaction of, with dibromopropane)
    50602-48-7P 52489-75-5P 52489-76-6P
ΙT
    52489-77-7P 52489-79-9P 52489-81-3P
    52489-83-5P 52489-85-7P 52489-87-9P
    52489-89-1P 52489-91-5P 52489-92-6P
    52489-93-7P 52489-94-8P 52489-95-9P
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52489-97-1P 52489-98-2P 52490-00-3P 52490-01-4P 52490-03-6P 52490-05-8P

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52490-06-9P 52490-07-0P 52490-08-1P
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     52490-17-2P 52490-19-4P 52490-21-8P
     52490-22-9P 52490-23-0P 52490-24-1P
     52490-25-2P 52490-27-4P 52490-28-5P
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     52490-68-3P 52490-72-9P 52490-74-1P
     52490-76-3P 52490-77-4P 52490-78-5P
     52490-79-6P 52490-80-9P 52490-81-0P
     52490-82-1P 52490-83-2P 52552-55-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     3265-74-5 52489-34-6 52489-41-5
ΤT
     52489-42-6 52489-43-7 52489-44-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (reaction of, with thionyl chloride)
     52489-45-9P 52489-46-0P 52489-47-1P
ΙT
     52489-48-2P 52489-49-3P 52489-50-6P
     52489-51-7P 52489-52-8P 52489-53-9P
     52489-54-0P 52489-55-1P 52489-56-2P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation and ether cleavage of)
     52489-45-9 CAPLUS
RN
CN
     Methanone, (2-ethyl-3-benzofuranyl)(4-methoxy-3,5-dimethylphenyl)- (CA
     INDEX NAME)
```

RN 52489-47-1 CAPLUS
CN Methanone, (4-methoxy-3,5-dimethylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-48-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(4-methoxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-49-3 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl)(2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-50-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(3,5-diethyl-4-methoxyphenyl)- (CA INDEX NAME)

$$\underbrace{ \begin{array}{c} \text{OMe} \\ \text{O} \\ \text{Et} \\ \end{array} }$$

RN 52489-51-7 CAPLUS

CN Methanone, (4-methoxy-3,5-dimethylphenyl)[2-(1-methylethyl)-3-benzofuranyl]- (CA INDEX NAME)

RN 52489-52-8 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)(4-methoxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-53-9 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-54-0 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl)(4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52489-55-1 CAPLUS

CN Methanone, (4-methoxy-3,5-dipropylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-56-2 CAPLUS CN Methanone, (2-butyl-3-benzofuranyl)(4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52489-71-1 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-diethylphenyl](2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-72-2 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-73-3 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-dipropylphenyl](2-propyl-3-benzofuranyl)- (CA INDEX NAME)

$$0 \longrightarrow Pr-n \qquad 0 \longrightarrow (CH2) 3 \longrightarrow Br$$

$$Pr-n$$

$$Pr-n$$

RN 52489-74-4 CAPLUS

CN Methanone, [4-(3-bromopropoxy)-3,5-dipropylphenyl](2-butyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-16-1 CAPLUS

CN Methanone, [4-(3-bromopropoxy)phenyl](2-butyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-52-5 CAPLUS

CN Methanone, [4-(4-bromobutoxy)phenyl](2-butyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-53-6 CAPLUS

CN Methanone, [4-(4-bromobutoxy)-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-61-6 CAPLUS

CN Methanone, [4-[(5-bromopentyl)oxy]phenyl](2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-62-7 CAPLUS

CN Methanone, [4-[(5-bromopentyl)oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-69-4 CAPLUS

CN Methanone, [4-[(6-bromohexyl)oxy]phenyl](2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52490-70-7 CAPLUS

CN Methanone, [4-[(6-bromohexyl)oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-36-8 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-methyl- (CA INDEX NAME)

RN 52489-37-9 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-propyl- (CA INDEX NAME)

$$\text{Pr-n} \\ \text{C-Cl}$$

RN 52489-38-0 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-(1-methylethyl)- (CA INDEX NAME)

RN 52489-39-1 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-butyl- (CA INDEX NAME)

$$\text{Su-n}$$

$$\text{C-cl}$$

RN 52489-40-4 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-cyclohexyl- (CA INDEX NAME)

ΙΤ

52489-58-4P 52489-59-5P 52489-60-8P

RN 52489-58-4 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl)(4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-59-5 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl)(2-methyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-60-8 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-61-9 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl)[2-(1-methylethyl)-3-benzofuranyl]- (CA INDEX NAME)

RN 52489-62-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-63-1 CAPLUS

CN Methanone, (3,5-diethyl-4-hydroxyphenyl)(2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-64-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(3,5-diethyl-4-hydroxyphenyl)- (CA INDEX NAME)

RN 52489-65-3 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)(4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-66-4 CAPLUS

CN Methanone, (3,5-diethyl-4-hydroxyphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-67-5 CAPLUS CN Methanone, (2-ethyl-3-benzofuranyl)(4-hydroxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52489-68-6 CAPLUS

CN Methanone, (4-hydroxy-3,5-dipropylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-69-7 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(4-hydroxy-3,5-dipropylphenyl)- (CA INDEX NAME)

IT 50602-48-7P 52489-75-5P 52489-76-6P 52489-77-7P 52489-79-9P 52489-81-3P 52489-83-5P 52489-85-7P 52489-87-9P 52489-89-1P 52489-91-5P 52489-92-6P 52489-93-7P 52489-94-8P 52489-95-9P 52489-97-1P 52489-98-2P 52490-00-3P 52490-01-4P 52490-03-6P 52490-05-8P

```
52490-06-9P 52490-07-0P 52490-08-1P
     52490-10-5P 52490-12-7P 52490-14-9P
     52490-17-2P 52490-19-4P 52490-21-8P
     52490-22-9P 52490-23-0P 52490-24-1P
     52490-25-2P 52490-27-4P 52490-28-5P
     52490-29-6P 52490-31-0P 52490-32-1P
     52490-33-2P 52490-35-4P 52490-36-5P
     52490-38-7P 52490-40-1P 52490-42-3P
     52490-44-5P 52490-46-7P 52490-48-9P
     52490-49-0P 52490-50-3P 52490-51-4P
     52490-55-8P 52490-56-9P 52490-58-1P
     52490-60-5P 52490-64-9P 52490-66-1P
     52490-68-3P 52490-72-9P 52490-74-1P
     52490-76-3P 52490-77-4P 52490-78-5P
     52490-79-6P 52490-80-9P 52490-81-0P
     52490-82-1P 52490-83-2P 52552-55-3P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
     50602-48-7 CAPLUS
RN
CN
    Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-
     benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)
```

● HCl

RN 52489-75-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl](2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 52489-76-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
& \text{Et} \\
& \text{O-} (CH_2) 3-N(Pr-n) 2 \\
& \text{Et}
\end{array}$$

● HCl

RN 52489-77-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl](2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{Pr-n} & \text{Et} \\
 & \text{O-} (CH_2) 3-N (Pr-n) 2 \\
 & \text{Et}
\end{array}$$

● HCl

RN 52489-79-9 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-78-8 CMF C33 H47 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-81-3 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-80-2 CMF C32 H45 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-83-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-82-4 CMF C34 H49 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-85-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-84-6 CMF C33 H47 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-87-9 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-86-8 CMF C35 H51 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-89-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-88-0 CMF C34 H49 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-91-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-90-4 CMF C36 H53 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-92-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52489-93-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
\text{Me} & \text{O-}(CH_2) \text{ } 3-N \text{ } (Pr-n) \text{ } 2\\
\text{Me} & \text{Me}
\end{array}$$

● HCl

RN 52489-94-8 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl](2-methyl-3-

benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O-}(CH_2) \text{ } 3-\text{N} \text{ } (Bu-n) \text{ } 2 \\ \hline \\ \text{Me} & \\ \end{array}$$

● HCl

RN 52489-95-9 CAPLUS

CN Methanone, [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52489-97-1 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(1-piperidinyl)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-96-0 CMF C27 H33 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52489-98-2 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl](2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O-}(\text{CH}_2) \text{ } 3-\text{N} \text{ } (\text{Pr-n}) \text{ } 2 \\ & \text{Me} & \\ \end{array}$$

● HCl

RN 52490-00-3 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl][2-(1-methylethyl)-3-benzofuranyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52489-99-3 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-01-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-03-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-02-5 CMF C32 H45 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-05-8 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-04-7 CMF C30 H41 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\mathbf{u} = \mathbf{u} = \mathbf{u}$$

RN 52490-06-9 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-07-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\underbrace{ \begin{array}{c} \text{Bu-n} \\ \text{C} \\ \end{array} } \underbrace{ \begin{array}{c} \text{Et} \\ \text{O- (CH2) 3-N (Bu-n) 2} \end{array}$$

● HCl

RN 52490-08-1 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl](2-ethyl-3-

benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-10-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]-3,5-diethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-09-2 CMF C30 H41 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-12-7 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-11-6 CMF C34 H47 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-14-9 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-13-8 CMF C32 H43 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-17-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-19-4 CAPLUS
CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3(dibutylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-18-3
CMF C32 H43 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-21-8 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylmethylamino)propoxy]phenyl], ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-20-7
CMF C27 H35 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-22-9 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-methyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 52490-23-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-ethyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 52490-24-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-propyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 52490-25-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

● HCl

RN 52490-27-4 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-28-5 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-29-6 CAPLUS
CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-31-0 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-30-9 CMF C28 H37 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-32-1 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(1-piperidinyl)propoxy]phenyl]-,
hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-33-2 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-35-4 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-34-3 CMF C28 H37 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-36-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

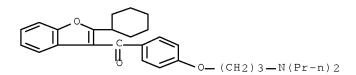
● HCl

RN 52490-38-7 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3- (dipropylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-37-6 CMF C30 H39 N O3



CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\underset{\mathsf{H} \circ -}{\overset{\circ}{\mathsf{U}}} = \overset{\circ}{\overset{\circ}{\mathsf{U}}} = \overset{\circ}{\circ} \mathsf{H}$$

RN 52490-40-1 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-39-8 CMF C28 H35 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-42-3 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-41-2 CMF C27 H35 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-44-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-propyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-43-4 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-46-7 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-45-6 CMF C26 H33 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-48-9 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dimethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
& \text{Me} \\
& \text{O-} (CH_2) 3-NMe_2 \\
& \text{Me}
\end{array}$$

● HCl

RN 52490-49-0 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-50-3 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-51-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dimethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$O = C + O =$$

● HCl

RN 52490-55-8 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(dipropylamino)butoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-54-7 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-56-9 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(1-piperidinyl)butoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-58-1 CAPLUS

CN Methanone, [4-[4-(dibutylamino)butoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-57-0 CMF C31 H43 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\mathbf{H} \circ \mathbf{H} \circ \mathbf{H} \circ \mathbf{H}$$

RN 52490-60-5 CAPLUS

CN Methanone, [4-[4-(dipropylamino)butoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-59-2 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-64-9 CAPLUS

CN Methanone, [4-[[5-(dipropylamino)pentyl]oxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-63-8 CMF C28 H37 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-66-1 CAPLUS

CN Methanone, [4-[[5-(dipropylamino)pentyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-65-0 CMF C30 H41 N O3

$$\begin{array}{c|c} & \text{Me} & \text{O-}(\text{CH2}) \text{ 5-N (Pr-n) 2} \\ & & \text{Me} \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\mathsf{H} \circ \mathbf{L} \overset{\circ}{\mathsf{L}} \overset{\circ}{\mathsf{L}} \overset{\circ}{\mathsf{L}} \circ \mathsf{H}$$

RN 52490-68-3 CAPLUS

CN Methanone, [4-[[5-(dibutylamino)pentyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-67-2 CMF C32 H45 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-72-9 CAPLUS

CN Methanone, [4-[[6-(dipropylamino)hexyl]oxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-71-8 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-74-1 CAPLUS

CN Methanone, [4-[[6-(dipropylamino)hexyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-73-0 CMF C31 H43 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-76-3 CAPLUS

CN Methanone, [4-[[6-(dibutylamino)hexyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52490-75-2 CMF C33 H47 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52490-77-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(propylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-78-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(methylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-79-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(ethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-80-9 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]phenyl](2-butyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-81-0 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(propylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-82-1 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-83-2 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-[(1-methylethyl)amino]propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52552-55-3 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylethylamino)propoxy]phenyl]-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 52552-54-2 CMF C28 H37 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

IT 3265-74-5 52489-34-6 52489-41-5 52489-42-6 52489-43-7 52489-44-8 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with thionyl chloride)

RN 3265-74-5 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-methyl- (CA INDEX NAME)

RN 52489-34-6 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-ethyl- (CA INDEX NAME)

RN 52489-41-5 CAPLUS

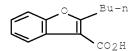
CN 3-Benzofurancarboxylic acid, 2-propyl- (CA INDEX NAME)

RN 52489-42-6 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-(1-methylethyl)- (CA INDEX NAME)

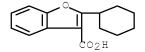
RN 52489-43-7 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-butyl- (CA INDEX NAME)



RN 52489-44-8 CAPLUS

CN 3-Benzofurancarboxylic acid, 2-cyclohexyl- (CA INDEX NAME)



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DOCUMENT NUMBER: 81:37442

ORIGINAL REFERENCE NO.: 81:5995a,5998a

TITLE: Benzofuran series. LIV. Potential antianginal

agents, 2-alkyl-3-(4-aminoalkoxy-3,5-dialkylbenzoyl)-

and 3-(4-aminoalkoxybenzoyl)benzofurans

AUTHOR(S): Gubin, J.; Claeys, N.; Deray, E.; Descamps, M.;

Bauthier, J.; Charlier, R.

CORPORATE SOURCE: Cent. Rech., S. A. Labaz N. V., Brussels, Belg.

SOURCE: European Journal of Medicinal Chemistry (1974), 9(1),

19-25

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE: Journal LANGUAGE: French

GI For diagram(s), see printed CA Issue.

Benzofurans I (R = Me, Et, Pr, CHMe2, Bu, cyclohexyl; R1 = H, Me, Et, Pr, CHMe2; R2 = R3 = Me, Et, Pr, Bu; R1 = H, R1 = Me, Et, Pr, CHMe2, Bu; R2 = Bu, R3 = Me, Et; NR2R3 = piperidino, 4-Me[Et, Pr, Ph]-piperazino; n = 3-6) were prepared by alkylating II. II (R1 = Me, Et, Pr, CHMe2) were prepared by treating the (chlorocarbonyl)benzofuran with dialkylanisoles and cleaving the Me ether with pyridine-HCl. I are antianginal, although I (R1 = Pr, CHMe2) were inactive. Some, especially I (R = Et, R1 = Me, R2 = R3 = Bu, n = 3), were more active than amiodarone.

CC 27-7 (Heterocyclic Compounds (One Hetero Atom))

IT 52489-58-4P 52489-59-5P 52489-60-8P 52489-61-9P 52489-62-0P 52489-63-1P 52489-64-2P 52489-65-3P 52489-66-4P 52489-67-5P 52489-68-6P 52489-69-7P

52901-28-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent) (preparation and aminoalkylation of)

(preparation and aminoalkylation (

IT 52489-35-7P 52489-36-8P 52489-37-9P 52489-38-0P 52489-39-1P 52489-40-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and arylation of)

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ΤТ
     52489-45-9P 52489-46-0P 52489-47-1P
     52489-48-2P 52489-49-3P 52489-50-6P
     52489-52-8P 52489-53-9P 52489-54-0P
     52489-55-1P 52489-56-2P 52901-64-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (preparation and demethylation of)
ΤТ
     3265-74-5P 50602-48-7P
                             52489-34-6P
                                            52489-41-5P 52489-42-6P
     52489-43-7P
                  52489-44-8P 52489-75-5P 52489-76-6P
     52489-77-7P 52489-92-6P 52489-93-7P
     52489-94-8P 52489-95-9P 52489-98-2P
     52490-01-4P 52490-06-9P 52490-07-0P
     52490-08-1P 52490-17-2P 52490-22-9P
     52490-23-0P 52490-24-1P 52490-25-2P
     52490-27-4P 52490-28-5P 52490-29-6P
     52490-32-1P 52490-33-2P 52490-36-5P
     52490-48-9P 52490-50-3P 52490-51-4P
     52490-56-9P 52490-77-4P 52490-78-5P
     52490-79-6P 52490-80-9P 52490-81-0P
     52490-82-1P 52490-83-2P 52901-30-1P
     52901-31-2P 52901-32-3P 52901-33-4P
     52901-34-5P 52901-35-6P 52901-36-7P
     52901-37-8P 52901-38-9P 52901-39-0P
     52901-40-3P 52901-41-4P 52901-42-5P
     52901-43-6P 52901-44-7P 52901-45-8P
     52901-46-9P 52901-48-1P 52901-49-2P
     52901-51-6P 52901-52-7P 52901-53-8P
     52901-54-9P 52901-55-0P 52901-56-1P
     52901-57-2P 52901-58-3P 52901-59-4P
     52956-64-6P 52956-65-7P 52956-66-8P
     52956-67-9P 52956-68-0P 52956-69-1P
     52956-70-4P 52956-71-5P 53049-34-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
ΙT
     52489-58-4P 52489-59-5P 52489-60-8P
     52489-61-9P 52489-62-0P 52489-63-1P
     52489-64-2P 52489-65-3P 52489-66-4P
     52489-67-5P 52489-68-6P 52489-69-7P
     52901-28-7P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP
     (Preparation); RACT (Reactant or reagent)
        (preparation and aminoalkylation of)
RN
     52489-58-4 CAPLUS
CN
     Methanone, (2-ethyl-3-benzofuranyl) (4-hydroxy-3,5-dimethylphenyl) - (CA
     INDEX NAME)
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RN 52489-59-5 CAPLUS
CN Methanone, (4-hydroxy-3,5-dimethylphenyl)(2-methyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-60-8 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-61-9 CAPLUS

CN Methanone, (4-hydroxy-3,5-dimethylphenyl)[2-(1-methylethyl)-3-benzofuranyl]- (CA INDEX NAME)

RN 52489-62-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-63-1 CAPLUS

CN Methanone, (3,5-diethyl-4-hydroxyphenyl)(2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-64-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(3,5-diethyl-4-hydroxyphenyl)- (CA INDEX NAME)

RN 52489-65-3 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)(4-hydroxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-66-4 CAPLUS

CN Methanone, (3,5-diethyl-4-hydroxyphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-67-5 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl)(4-hydroxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52489-68-6 CAPLUS
CN Methanone, (4-hydroxy-3,5-dipropylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-69-7 CAPLUS CN Methanone, (2-butyl-3-benzofuranyl)(4-hydroxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52901-28-7 CAPLUS
CN Methanone, (2-ethyl-3-benzofuranyl)[4-hydroxy-3,5-bis(1-methylethyl)phenyl]- (CA INDEX NAME)

RN 52489-36-8 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-methyl- (CA INDEX NAME)

RN 52489-37-9 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-propyl- (CA INDEX NAME)

RN 52489-38-0 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-(1-methylethyl)- (CA INDEX NAME)

RN 52489-39-1 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-butyl- (CA INDEX NAME)

$$\text{C-Cl}$$

RN 52489-40-4 CAPLUS

CN 3-Benzofurancarbonyl chloride, 2-cyclohexyl- (CA INDEX NAME)

$$\bigcap_{C} \bigcap_{C \subset C} C$$

RN 52489-46-0 CAPLUS

CN Methanone, (4-methoxy-3,5-dimethylphenyl)(2-methyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-47-1 CAPLUS

CN Methanone, (4-methoxy-3,5-dimethylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-48-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(4-methoxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-49-3 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl)(2-ethyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-50-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(3,5-diethyl-4-methoxyphenyl)- (CA INDEX NAME)

RN 52489-52-8 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)(4-methoxy-3,5-dimethylphenyl)- (CA INDEX NAME)

RN 52489-53-9 CAPLUS

CN Methanone, (3,5-diethyl-4-methoxyphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-54-0 CAPLUS

CN Methanone, (2-ethyl-3-benzofuranyl)(4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52489-55-1 CAPLUS

CN Methanone, (4-methoxy-3,5-dipropylphenyl)(2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 52489-56-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)(4-methoxy-3,5-dipropylphenyl)- (CA INDEX NAME)

RN 52901-64-1 CAPLUS
CN Methanone, (2-ethyl-3-benzofuranyl)[4-methoxy-3,5-bis(1-methylethyl)phenyl]- (CA INDEX NAME)

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50602-48-7P 52489-75-5P 52489-76-6P
ΙT
     52489-77-7P 52489-92-6P 52489-93-7P
     52489-94-8P 52489-95-9P 52489-98-2P
     52490-01-4P 52490-06-9P 52490-07-0P
     52490-08-1P 52490-17-2P 52490-22-9P
     52490-23-0P 52490-24-1P 52490-25-2P
     52490-27-4P 52490-28-5P 52490-29-6P
     52490-32-1P 52490-33-2P 52490-36-5P
     52490-48-9P 52490-50-3P 52490-51-4P
     52490-56-9P 52490-77-4P 52490-78-5P
     52490-79-6P 52490-80-9P 52490-81-0P
     52490-82-1P 52490-83-2P 52901-30-1P
     52901-31-2P 52901-32-3P 52901-33-4P
     52901-34-5P 52901-35-6P 52901-36-7P
     52901-37-8P 52901-38-9P 52901-39-0P
     52901-40-3P 52901-41-4P 52901-42-5P
     52901-43-6P 52901-44-7P 52901-45-8P
     52901-46-9P 52901-48-1P 52901-49-2P
     52901-51-6P 52901-52-7P 52901-53-8P
     52901-54-9P 52901-55-0P 52901-56-1P
     52901-57-2P 52901-58-3P 52901-59-4P
     52956-64-6P 52956-65-7P 52956-66-8P
     52956-67-9P 52956-68-0P 52956-69-1P
     52956-70-4P 52956-71-5P 53049-34-6P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
RN
     50602-48-7 CAPLUS
CN
    Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-
     benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)
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$$\begin{array}{c} \text{Me} \\ \text{O} \\ \text{C} \\ \text{Me} \end{array}$$

● HCl

RN 52489-75-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl](2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O-}(\text{CH}_2) \text{ } 3-\text{N} \text{ } (\text{Bu-n}) \text{ } 2 \\ & \text{Me} & \text{Me} \\ \end{array}$$

● HCl

RN 52489-76-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
& \text{Bu-n} & \text{Et} \\
& \text{O-} (CH_2) 3-N (Pr-n) 2 \\
& \text{Et}
\end{array}$$

● HCl

RN 52489-77-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl](2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
& \text{Et} \\
& \text{O-} (CH_2) 3-N (Pr-n) 2 \\
& \text{Et}
\end{array}$$

● HCl

RN 52489-92-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{O-}(CH_2) \text{ } 3-\text{N}(Pr-n) \text{ } 2 \\ \hline & \text{Me} & \\ & \text{Me} & \\ \end{array}$$

● HCl

RN 52489-93-7 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
\text{Me} & \text{O-}(CH_2) 3-N(Pr-n) 2 \\
\text{Me} & \text{Me}
\end{array}$$

● HCl

RN 52489-94-8 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52489-95-9 CAPLUS

CN Methanone, [4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52489-98-2 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl](2-propyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-01-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
& \text{Me} \\
& \text{O-} (CH_2) 3 - NEt_2 \\
& \text{Me}
\end{array}$$

● HCl

RN 52490-06-9 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-diethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-07-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-08-1 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-17-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 52490-22-9 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-methyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 52490-23-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-ethyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 52490-24-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-propyl-1-piperazinyl)propoxy]phenyl]-, dihydrochloride (9CI) (CA INDEX NAME)

●2 HC1

RN 52490-25-2 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

● HCl

RN 52490-27-4 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-28-5 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-29-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-32-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(1-piperidinyl)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-33-2 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-methyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-36-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-48-9 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dimethylamino)propoxy]-3,5-dimethylphenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
& \text{Me} \\
& \text{O-} (CH_2) 3-NMe_2 \\
& \text{Me}
\end{array}$$

● HCl

RN 52490-50-3 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl][2-(1-methylethyl)-3-benzofuranyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O & CH2 \end{array}$$

● HCl

RN 52490-51-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dimethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

● HCl

RN 52490-56-9 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(1-piperidinyl)butoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 52490-77-4 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(propylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-78-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(methylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-79-6 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(ethylamino)propoxy]phenyl]-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-80-9 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]phenyl](2-butyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-81-0 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(propylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-82-1 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52490-83-2 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-[(1-methylethyl)amino]propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52901-30-1 CAPLUS

CN Methanone, [4-[4-(dipropylamino)butoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-59-2 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-31-2 CAPLUS
CN Methanone, [4-[4-(dibutylamino)butoxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-57-0
CMF C31 H43 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-32-3 CAPLUS

CN Methanone, [4-[[5-(dipropylamino)pentyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-65-0 CMF C30 H41 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\mathbf{H} \circ \mathbf{U} \circ \mathbf{U} \circ \mathbf{H}$$

RN 52901-33-4 CAPLUS

CN Methanone, [4-[[6-(dipropylamino)hexyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-73-0 CMF C31 H43 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-34-5 CAPLUS

CN Methanone, [4-[[6-(dibutylamino)hexyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-75-2 CMF C33 H47 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-35-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl][2-(1-methylethyl)-3-benzofuranyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-99-3 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-36-7 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl) [4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-04-7 CMF C30 H41 N O3

$$\begin{array}{c|c} & \text{Me} & \text{O-}(\text{CH2}) \text{ 3-N}(\text{Pr-n}) \text{ 2} \\ & & \text{Me} \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-37-8 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-13-8 CMF C32 H43 N O3

$$\begin{array}{c|c} O & \\ \hline \\ O & \\ \hline \\ Me \end{array} \\ \begin{array}{c} Me \\ \hline \\ O - (CH_2) \ 3 - N(Pr-n) \ 2 \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-38-9 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-11-6 CMF C34 H47 N O3

$$\begin{array}{c|c}
 & \text{Me} \\
 & \text{O} \quad \text{(CH2)} \ 3-\text{N(Bu-n)} \ 2
\end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-39-0 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-diethylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-78-8 CMF C33 H47 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-40-3 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]-3,5-diethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-09-2
CMF C30 H41 N O3

CM 2

CRN 144-62-7

CMF C2 H2 O4

RN 52901-41-4 CAPLUS
CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-80-2 CMF C32 H45 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-42-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-82-4 CMF C34 H49 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-43-6 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-84-6 CMF C33 H47 N O3

$$\begin{array}{c|c}
 & \text{O-CH2} & 3-N \text{ (Pr-n) 2} \\
 & \text{Pr-n} & \text{Pr-n}
\end{array}$$

```
10/584440
```

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-44-7 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl](2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-86-8 CMF C35 H51 N O3

$$\begin{array}{c|c}
 & \text{O-CH2} & \text{3-N(Bu-n)} & 2 \\
 & \text{Pr-n} & \text{Pr-n}
\end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-45-8 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-90-4 CMF C36 H53 N O3

$$\begin{array}{c|c}
& \text{N-Pr} \\
& \text{O-} (CH2) 3-N (Bu-n) 2 \\
& \text{Pr-n}
\end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-46-9 CAPLUS

CN Methanone, [4-[3-(dipropylamino)propoxy]-3,5-bis(1-methylethyl)phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52901-48-1 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]-3,5-bis(1-methylethyl)phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52901-47-0 CMF C34 H49 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-49-2 CAPLUS

CN Methanone, [3,5-bis(1-methylethyl)-4-[3-(1-piperidinyl)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 52901-51-6 CAPLUS

CN Methanone, [4-[3-(dimethylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52901-50-5 CMF C22 H25 N O3

$$\begin{array}{c} \text{Et} \\ \text{C} \\ \text{C} \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\text{HO} = \bigcup_{i=0}^{\infty} \bigcup_{j=0}^{\infty} \bigcup_{i=0}^{\infty}$$

RN 52901-52-7 CAPLUS
CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-34-3
CMF C28 H37 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-53-8 CAPLUS
CN Methanone, [4-[3-(dipropylamino)propoxy]phenyl](2-propyl-3-benzofuranyl)-,
 ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-41-2 CMF C27 H35 N O3

CM 2

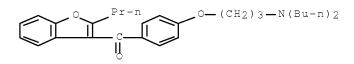
CRN 144-62-7 CMF C2 H2 O4

RN 52901-54-9 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-propyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-43-4 CMF C29 H39 N O3



CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52901-55-0 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-45-6 CMF C26 H33 N O3

CM 2

CRN 144-62-7

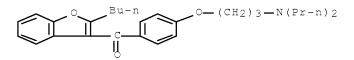
CMF C2 H2 O4

RN 52901-56-1 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-30-9 CMF C28 H37 N O3



CM 2

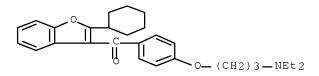
CRN 144-62-7 CMF C2 H2 O4

RN 52901-57-2 CAPLUS

CN Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-39-8 CMF C28 H35 N O3



```
CM
          2
     CRN 144-62-7
     CMF C2 H2 O4
 но_0_0_0
     52901-58-3 CAPLUS
RN
CN
    Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-
     (dipropylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)
     CM
     CRN 52490-37-6
     CMF C30 H39 N O3
                       O = (CH2) 3 - N(Pr-n) 2
     CM
          2
     CRN 144-62-7
     CMF C2 H2 O4
     52901-59-4 CAPLUS
RN
    Methanone, (2-cyclohexyl-3-benzofuranyl)[4-[3-
     (dibutylamino)propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)
     CM
          1
     CRN 52490-18-3
     CMF C32 H43 N O3
```

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52956-64-6 CAPLUS

CN Methanone, [4-[[5-(dibutylamino)pentyl]oxy]-3,5-dimethylphenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-67-2 CMF C32 H45 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52956-65-7 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]-3,5-dimethylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-02-5 CMF C32 H45 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52956-66-8 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(dipropylamino)propoxy]-3,5-dipropylphenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-88-0 CMF C34 H49 N O3

CM 2

$$\mathsf{HO} = \bigcup_{\mathsf{H}}^{\mathsf{O}} = \bigcup_{\mathsf{H}}^{\mathsf{O}} = \mathsf{OH}$$

RN 52956-67-9 CAPLUS
CN Methanone, [4-[[5-(dipropylamino)pentyl]oxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-63-8
CMF C28 H37 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 52956-68-0 CAPLUS
CN Methanone, [4-[[6-(dipropylamino)hexyl]oxy]phenyl](2-ethyl-3-benzofuranyl), ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-71-8
CMF C29 H39 N O3

CM 2

RN 52956-69-1 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylmethylamino)propoxy]phenyl], ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-20-7
CMF C27 H35 N O3

CM 2

CRN 144-62-7

CMF C2 H2 O4

RN 52956-70-4 CAPLUS
CN Methanone, (2-butyl-3-benzofuranyl)[4-[3-(butylethylamino)propoxy]phenyl], ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52552-54-2
CMF C28 H37 N O3

CM 2

RN 52956-71-5 CAPLUS

CN Methanone, (2-butyl-3-benzofuranyl)[4-[4-(dipropylamino)butoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52490-54-7 CMF C29 H39 N O3

CM 2

CRN 144-62-7 CMF C2 H2 O4

$$\mathbf{H} = \mathbf{H} = \mathbf{H} = \mathbf{H}$$

RN 53049-34-6 CAPLUS

CN Methanone, [3,5-dimethyl-4-[3-(1-piperidinyl)propoxy]phenyl](2-ethyl-3-benzofuranyl)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 52489-96-0 CMF C27 H33 N O3

CM 2

```
=> d his full
     (FILE 'HOME' ENTERED AT 10:28:42 ON 19 FEB 2008)
    FILE 'REGISTRY' ENTERED AT 10:28:53 ON 19 FEB 2008
      STRUCTURE UPLOADED
L1
L2
            50 SEA SSS SAM L1
     FILE 'STNGUIDE' ENTERED AT 10:30:21 ON 19 FEB 2008
    FILE 'CASREACT' ENTERED AT 10:33:31 ON 19 FEB 2008
               STRUCTURE UPLOADED
1.3
L4
             0 SEA SSS SAM L3 ( 0 REACTIONS)
     FILE 'REGISTRY' ENTERED AT 10:35:51 ON 19 FEB 2008
              D STAT QUE L2
L5
         8858 SEA SSS FUL L1
                SAVE TEMP L5 CHA440STR1L/A
    FILE 'CASREACT' ENTERED AT 10:36:26 ON 19 FEB 2008
           324 SEA ABB=ON PLU=ON L5
L6
              0 SEA SUB=L6 SSS SAM L3 ( 0 REACTIONS) 2 SEA SUB=L6 SSS FUL L3 ( 8 REACTIONS)
L7
L8
                D SCA
   FILE 'REGISTRY' ENTERED AT 10:37:52 ON 19 FEB 2008
           STRUCTURE UPLOADED
L9
L10
              STRUCTURE UPLOADED
           50 SEA SUB=L5 SSS SAM L9
L11
          1802 SEA SUB=L5 SSS FUL L9
L12
L13
           50 SEA SUB=L5 SSS SAM L10
L14
          7056 SEA SUB=L5 SSS FUL L10
L15
            O SEA ABB=ON PLU=ON L12 AND L13
             O SEA ABB=ON PLU=ON L12 AND L14
L16
    FILE 'CAPLUS' ENTERED AT 10:40:32 ON 19 FEB 2008
L17
           230 SEA ABB=ON PLU=ON L12 (L) PREP/RL
            312 SEA ABB=ON PLU=ON L14 (L) (RACT OR RGT OR RCT)/RL 5 SEA ABB=ON PLU=ON L17 AND L18
L18
L19
L20
             O SEA ABB=ON PLU=ON SHOUTTEETEN A?/AU
L21
             4 SEA ABB=ON PLU=ON BLEGER F?/AU
             2 SEA ABB=ON PLU=ON MORDACO F?/AU
           66 SEA ABB=ON PLU=ON PIRON J?/AU
L23
             1 SEA ABB=ON PLU=ON L21 AND L22 AND L23
L24
               D AU
L25
             O SEA ABB=ON PLU=ON SCHOUTEETAN A?/AU
L26
            37 SEA ABB=ON PLU=ON SCHOUTEETEN A?/AU
L27
             2 SEA ABB=ON PLU=ON L21 AND (L22 OR L23 OR L26)
L28
             2 SEA ABB=ON PLU=ON L22 AND (L23 OR L26)
L29
             1 SEA ABB=ON PLU=ON L23 AND L26
             3 SEA ABB=ON PLU=ON (L27 OR L28 OR L29)
1 SEA ABB=ON PLU=ON L19 AND (L21 OR L22 OR L23 OR L26)
2 SEA ABB=ON PLU=ON L8
L30
L31
L32
L33
             1 SEA ABB=ON PLU=ON L32 AND (L21 OR L22 OR L23 OR L26)
                SEL AN
   FILE 'CASREACT' ENTERED AT 10:44:31 ON 19 FEB 2008
           1 SEA ABB=ON PLU=ON ("143:97254"/AN OR "2005:569050"/AN)
L34
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L35 1 SEA ABB=ON PLU=ON L34 AND L8

FILE 'REGISTRY' ENTERED AT 10:45:40 ON 19 FEB 2008

FILE 'CAPLUS' ENTERED AT 10:45:42 ON 19 FEB 2008

D STAT QUE L30 D STAT QUE L31

L36 3 SEA ABB=ON PLU=ON L30 OR L31

FILE 'CASREACT' ENTERED AT 10:46:02 ON 19 FEB 2008
D STAT OUE L35

FILE 'CAPLUS' ENTERED AT 10:46:58 ON 19 FEB 2008 D IBIB ABS HITSTR L36 1-3

FILE 'CASREACT' ENTERED AT 10:46:59 ON 19 FEB 2008
D IBIB ABS HIT L35 1

FILE 'REGISTRY' ENTERED AT 10:47:22 ON 19 FEB 2008

FILE 'CAPLUS' ENTERED AT 10:47:24 ON 19 FEB 2008
D STAT QUE L19

L37 4 SEA ABB=ON PLU=ON L19 NOT L36

FILE 'CASREACT' ENTERED AT 10:47:51 ON 19 FEB 2008 D STAT QUE L8

L38 1 SEA ABB=ON PLU=ON L8 NOT L35

FILE 'CASREACT, CAPLUS' ENTERED AT 10:48:16 ON 19 FEB 2008
L39 5 DUP REM L38 L37 (0 DUPLICATES REMOVED)

ANSWER '1' FROM FILE CASREACT

ANSWERS '2-5' FROM FILE CAPLUS

D IBIB ABS HIT L39 1

D IBIB ABS HITIND HITSTR L39 2-5

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7 DICTIONARY FILE UPDATES: 18 FEB 2008 HIGHEST RN 1004360-55-7

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http://www.cas.org/support/stngen/stndoc/properties.html

FILE STNGUIDE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Feb 15, 2008 (20080215/UP).

FILE CASREACT

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FILE CONTENT: 1840 - 16 Feb 2008 VOL 148 ISS 8

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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